Test of dilute gas approximation in quantum mechanical model

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(February 1, 2008)

Abstract

The validity of dilute gas approximation is explored by making use of the large-sized instanton in quantum mechanical model. It is shown that the Euclidean probability amplitude derived through a dilute gas approximation not only cannot explain the result of the linear combination of atomic orbitals approximation, but also does not exhibit a proper limiting case when the size of instanton is very large.

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It is well known that instanton method is a useful tool for the quantitative understanding of quantum tunneling[1, 2]. Although this method cannot inevitably avoid the Gaussian approximation, which is a common feature of path-integral formalism, in the course of evaluation of quantum fluctuation, it is believed that the multi-instanton contribution compensates the Euclidean probability amplitude for the information loss resulted from this approximation to a large extent. First successful result about this is reported by E. Gildener and A. Patrascioiu[3] in the quantum tunneling problem of double well potential. After treating the zero mode carefully, they calculated the multi-instanton contribution by using a dilute gas approximation. Comparing their result with that of linear combination of atomic orbitals(LCAO) approximation[4], they proved that their method provides a reasonable energy splitting, ΔE, due to tunneling effect. Recently it is shown that the repeat of the same procedure in a triple well potential case also gives a LCAO-type energy splitting[5].

Giving a very reasonable result in the quantum mechanical tunneling problem, the dilute instanton gas approximation gets some doubt in the scale invariant theory like the real dimensional QCD. This is because scale invariance makes the instanton size not to be determined. In the real dimensional QCD the large size of instanton gives rise to a troublesome infrared problem in the θ-vacuum energy. Although several different approaches[6, 7, 8] are suggested in order to escape from this difficulty, the result does not seem to be conclusive.

In this paper we will examine the validity of a dilute gas approximation and explore the information loss due to this approximation by introducing the large-sized instanton in the simple quantum mechanical model. The large-sized instanton, which is essential for the test of the dilute gas approximation, is easily produced by using a potential

$$V(\phi) = \alpha(\phi^2 + \gamma)(\phi - \beta)^2(\phi + \beta)^2 \tag{1}$$

where $\gamma > 0$. An interesting feature of the potential (1) is that it can be either double well or triple well depending on the values of γ and β as shown in Fig.1. In the double well region $(\gamma > \frac{\beta^2}{2})$, it is well known that the LCAO approximation results in

$$\lim_{T \to \infty} < \phi_f, T \mid \phi_i, -T > \propto < \phi_f \mid R_0 >< L_0 \mid \phi_i > e^{-2E_0 T} \sinh(2\Delta E T) \tag{2}$$

where E_0 and ΔE are the unperturbed vacuum energy and half of energy splitting, respectively, and $\mid R_0 >$ and $\mid L_0 >$ denote the normalized lowest energy eigenstates of the isolated wells. For the small γ case($\gamma \ll \frac{\beta^2}{2}$), the central false vacuum holds off the transition from left true vacuum to right one and makes the large-sized instanton as a result of this fact. The smaller γ is, the larger instanton we can get. In this case the LCAO approximation gives

$$\lim_{T \to \infty} < \phi_f, T \mid \phi_i, -T > \tag{3}$$
$$= < \phi_f \mid R_0 >< L_0 \mid \phi_i > \left[\frac{e^{-2E_0'T}}{2 + a_+^2} + \frac{e^{-2E_2'T}}{2 + a_-^2} - \frac{1}{2}e^{-2E_1'T} \right]$$

where $a_\pm$ and $E_n'(n = 0, 1, 2)$ are given in Ref.[5]. So it is very easy to show that $\lim_{T \to \infty} < \phi_f, T \mid \phi_i, -T >$ cannot contain the hyperbolic-sine term in this case.

Now let us calculate the same quantity by following the usual instantonic procedure. By integrating the Euclidean equation of motion

$$\frac{1}{2}(\frac{d\phi}{d\tau})^2 = \alpha(\phi^2 + \gamma)(\phi - \beta)^2(\phi + \beta)^2 \tag{4}$$

the instanton solution and corresponding classical Euclidean action for large T are straightforwardly derived after a tedious calculation:

$$\phi_{cl} = \epsilon(\tau - \tau_0)\beta\sqrt{\frac{\cosh[2\sqrt{2\alpha(\beta^2 + \gamma)}\beta(\tau - \tau_0)] - 1}{\cosh[2\sqrt{2\alpha(\beta^2 + \gamma)}\beta(\tau - \tau_0)] + \frac{2\beta^2 + \gamma}{\gamma}}} \tag{5}$$
$$S_{cl} = \sqrt{\alpha}\beta^3 \frac{(\beta^2 + \gamma)^{5/2}}{\gamma^2} \frac{\Gamma(\frac{11}{4})}{\Gamma(\frac{5}{2})\Gamma(\frac{1}{4})} F(3, \frac{5}{2}; \frac{11}{4}; -\frac{\beta^2}{\gamma})$$

where $\epsilon(x)$ and $F(a, b; c; z)$ are usual alternating and hypergeometric functions.

By defining the change of variable

$$\phi = \phi_{cl} + \eta \tag{6}$$

one instanton contribution to the Euclidean probability amplitude becomes

$$< \phi_f, T \mid \phi_i, -T >= e^{-S_{cl}}I_1(T) \tag{7}$$

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where

$$I_1(T) = \int_{(-T,0)}^{(T,0)} D\eta e^{-\int d\tau \eta \hat{M} \eta} \tag{8}$$

and

$$\hat{M} = -\frac{1}{2}\frac{d^2}{d\tau^2} + \alpha[15\phi_{cl}^4 - 6(2\beta^2 - \gamma)\phi_{cl}^2 + \beta^2(\beta^2 - 2\gamma)]. \tag{9}$$

It is straightforward to prove that $\dot{\phi}_{cl} \equiv \frac{d\phi_{cl}}{d\tau}$ is zero mode of $\hat{M}$. The repeat of the procedure given in Ref.[3] enables one to get the one instanton contribution of the Euclidean amplitude as

$$< \phi_f, T \mid \phi_i, -T >_{(1)} = e^{-S_{cl}}\frac{16T}{\pi}\frac{\beta^3(\beta^2 + \gamma)^2 2\alpha}{\gamma}e^{-2\sqrt{2\alpha(\beta^2 + \gamma)}\beta T} \tag{10}$$

where the subscript (1) means the one instanton contribution.

The multi-instanton contribution to the probability amplitude can be obtained by summing the possible configurations and using a dilute gas approximation:

$$< \phi_f, T \mid \phi_i, -T > \tag{11}$$
$$= \sqrt{\frac{\omega}{\pi}}e^{-\omega T}\sum_{n=0}^{\infty}\frac{1}{(2n+1)!}\left[e^{-S_{cl}}\frac{16T}{\sqrt{\pi\omega}}\frac{\beta^3(\beta^2 + \gamma)^2 2\alpha}{\gamma}\right]^{2n+1}$$
$$= \sqrt{\frac{2\sqrt{2\alpha(\beta^2 + \gamma)}\beta}{\pi}}e^{-2\sqrt{2\alpha(\beta^2 + \gamma)}\beta T}\sinh\left[e^{-S_{cl}}\frac{16T}{\sqrt{2\pi}}\frac{(2\alpha)^{3/4}\beta^{5/2}(\beta^2 + \gamma)^{7/4}}{\gamma}\right]$$

where $\omega = 2\sqrt{2\alpha(\beta^2 + \gamma)}\beta$. In Eq.(11) the most dominant instanton density in the summation is

$$\frac{n}{T} \sim e^{-\frac{S_{cl}}{\hbar}}\frac{16}{\sqrt{\pi\omega}}\frac{\beta^3(\beta^2 + \gamma)^2 2\alpha}{\gamma} \tag{12}$$

where the Plank constant $\hbar$ in the exponent is explicitly expressed for the following remark.

Since the classical Euclidean action S_{cl} is finite in the double well region, the dominant instanton density becomes very small, which guarantees the justification of the dilute gas approximation. By comparing Eq.(11) with (2) one can read

$$E_0 = \sqrt{2\alpha(\beta^2 + \gamma)}\beta \tag{13}$$
$$\Delta E = \frac{8}{\sqrt{2\pi}}\frac{(2\alpha)^{3/4}\beta^{5/2}(\beta^2 + \gamma)^{7/4}}{\gamma}e^{-S_{cl}}$$

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in this region. If γ increases, $\Delta E \propto \gamma^{\frac{3}{4}} e^{-c_1 \gamma^{1/2}}$, where c_1 is some constant, goes to zero which is physically reasonable.

However, situation is quite different in the small γ region. In this region one can easily show

$$S_{cl} = c_2 \gamma^{\frac{1}{2}}, \tag{14}$$

where c_2 is a γ-independent constant, by invoking the asymptotic formula of hypergeometric function. If γ is less than or order of $(\hbar/c_2)^2$, Eq.(12) casts a doubt on the validity of the dilute gas approximation in this region. As expected, the probability amplitude derived through dilute gas approximation

$$< \phi_f, T \mid \phi_i, -T > \propto \sinh\left[e^{-S_{cl}} \frac{16T}{\sqrt{2\pi}} \frac{(2\alpha)^{3/4} \beta^6}{\gamma} \right]. \tag{15}$$

cannot explain the LCAO result (3). The worse fact in this region is that $\gamma = 0$ limit of Eq.(15) is not well-defined although the potential is rarely changed from $\alpha \phi^2 (\phi - \beta)^2 (\phi + \beta)^2$. This means that multi-instanton contribution calculated through the dilute gas approximation loses too much information when the size of instanton is very large. Although one can see the breakdown of dilute gas approximation in the strong coupling region of the double well case[9], the origin of the breakdown is quite different in this case. The origin of this phenomena in this case seems to be the sensitivity and large size of classical solution.

In this stage the following natural and fundamental question arises: Is there any other approximation method which replaces the dilute gas approximation and is able to explain LCAO result regardless of the instanton size? Although the model presented in this paper is not scale invariant, the investigation of the answer of the above question in this simple quantum mechanical model may shed light on the complicated QCD problem.

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FIGURES

FIG. 1. potential (1) at double well and triple well regions